Efficient Multirate Methods from High Order

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Introduction

- Multiphysics applications have specific coupling properties:
  - Coupled in the bulk (magnetohydrodynamics, cosmology)
  - Coupled across interfaces (climate, tokamaks)
- Multiphysics simulation challenges include:
  - Multirate processes, but too close to analytically reformulate.
  - Optimal solvers may exist for some pieces, but not for the whole.
  - Mixing of stiff/nonstiff processes, challenging standard solvers.
- Many legacy codes utilize lowest-order time step splittings, may suffer from:
  - Low accuracy typically O(h)-accurate; symmetrization/extrapolation may improve this but at significant cost [Ropp, Shadid & Ober 2005].
  - Poor/unknown stability even when each part utilizes a stable step size, the combined problem may admit unstable modes [Estep et al., 2007].

Need for Flexible High-Order Multirate Integrators

Multirate methods evolve distinct problem components with their own rate-specific time steps.

- Historical approaches:
  - Simple (h)-accurate subcycling approaches
  - Interpolation to handle fast/slow coupling (typically (h^2) , sometimes (h^3)) [Kværnø & Rentrop, 1999; . . .].
  - Extrapolation methods to bootstrap accuracy for low order methods [Engstler & Lubich, 1997; Constantinescu & Sandu, 2013; . . .].
- Next-generation methods will require a variety of criteria:
  - High-order accuracy stability, both within and between components
  - Flexible rate structure within integration, or even to dynamically identify fast vs slow partitioning of components
  - Robust temporal error estimation adaptivity of step size(s)
  - Enable problem-specific options, e.g. SSP or symplectic for specific components

GARK framework for 2-rate problem

- Consider:

$\mathbf{A}^{\{f,f\}}$	$\mathbf{A}^{\{f,s\}}$
$\mathbf{A}^{\{s,f\}}$	$\mathbf{A}^{\{s,s\}}$
$\mathbf{b}^{\{f\}\intercal}$	$\mathbf{b}^{\{s\}\intercal}$

- General: $\frac{dy}{dt} = F(t,y), \quad y(t_0) = y_0$
  - $F(t,y)$ with fast portion and a slow portion
  - slow time-step size h, fast time-step size h/m
  - time-scale separation m

- Additive:

$$y'(t) = F(t,y), \quad F(t,y) = f_f(t,y) + f_s(t,y), \quad t \geq t_0, \quad y(t_0) = y_0$$

- Stage and Solution Updates:

$$\mathbf{k}_j^{\{f\}} = \mathbf{y}_n + h\sum_{l=1}^{\mathbf{s}^{\{f\}}} a_{j,l}^{\{f,f\}} f^{\{f\}}\left(t_n + c_l^{\{f\}}h, \mathbf{k}_l^{\{f\}}\right) + h\sum_{l=1}^{\mathbf{s}^{\{s\}}} a_{j,l}^{\{f,s\}} f^{\{s\}}\left(t_n + c_l^{\{s\}}h, \mathbf{k}_l^{\{s\}}\right)$$

$$\mathbf{k}_i^{\{s\}} = \mathbf{y}_n + h\sum_{l=1}^{\mathbf{s}^{\{f\}}} a_{i,l}^{\{s,f\}} f^{\{f\}}\left(t_n + c_l^{\{f\}}h, \mathbf{k}_l^{\{f\}}\right) + h\sum_{l=1}^{\mathbf{s}^{\{s\}}} a_{i,l}^{\{s,s\}} f^{\{s\}}\left(t_n + c_l^{\{s\}}h, \mathbf{k}_l^{\{s\}}\right)$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\sum_{l=1}^{\mathbf{s}^{\{f\}}} b_l^{\{f\}} f^{\{f\}}\left(t_n + c_l^{\{f\}}h, \mathbf{k}_l^{\{f\}}\right) + h\sum_{l=1}^{\mathbf{s}^{\{s\}}} b_l^{\{s\}} f^{\{s\}}\left(t_n + c_l^{\{s\}}h, \mathbf{k}_l^{\{s\}}\right)$$

- Row-sum conditions give stage times: $c_j^{\{f\}} = \sum_{l=1}^{\mathbf{s}^{\{f\}}} a_{jl}^{\{f,f\}} = \sum_{l=1}^{\mathbf{s}^{\{s\}}} a_{jl}^{\{f,s\}}$ $\quad c_j^{\{s\}} = \sum_{l=1}^{\mathbf{s}^{\{s\}}} a_{jl}^{\{s,s\}} = \sum_{l=1}^{\mathbf{s}^{\{f\}}} a_{jl}^{\{s,f\}}$

GARK h^4 Order Conditions

For $\sigma, \nu, \mu \in \{f, s\}$, and assuming $\mathbf{c}^{\{\sigma\}} = \mathbf{A}^{\{\sigma,f\}}1^{\{f\}} = \mathbf{A}^{\{\sigma,s\}}1^{\{s\}}$:

$$
\begin{aligned}
\mathbf{b}^{\{\sigma\}\intercal}1^{\{\sigma\}} &= 1, & \mathbf{b}^{\{\sigma\}\intercal}\mathbf{c}^{\{\sigma\}} &= \frac{1}{2} & [h, h^2] \\
\mathbf{b}^{\{\sigma\}\intercal}\left(\mathbf{c}^{\{\sigma\}}\right)^2 &= \frac{1}{3}, & \mathbf{b}^{\{\sigma\}\intercal}\mathbf{A}^{\{\sigma,\nu\}}\mathbf{c}^{\{\nu\}} &= \frac{1}{6} & [h^3] \\
\mathbf{b}^{\{\sigma\}\intercal}\left(\mathbf{c}^{\{\sigma\}}\right)^3 &= \frac{1}{4}, & \left(\mathbf{b}^{\{\sigma\}}\times\mathbf{c}^{\{\sigma\}}\right)^\intercal\mathbf{A}^{\{\sigma,\nu\}}\mathbf{c}^{\{\nu\}} &= \frac{1}{8} & [h^4] \\
\mathbf{b}^{\{\sigma\}\intercal}\mathbf{A}^{\{\sigma,\nu\}}\left(\mathbf{c}^{\{\nu\}}\right)^2 &= \frac{1}{12}, & \mathbf{b}^{\{\sigma\}\intercal}\mathbf{A}^{\{\sigma,\mu\}}\mathbf{A}^{\{\mu,\nu\}}\mathbf{c}^{\{\nu\}} &= \frac{1}{24}. &
\end{aligned}
$$

Here, exponentiation and $\times$ denote component-wise operators.

We'll refer to these as "fast" conditions when $\sigma = f$ (and "slow" when $\sigma = s$).

As expected, the number of conditions increases dramatically with order: 2 for h, 4 for h^2 10 for h^3, and 28 for h^4 (note: h^5 has 86).

MIS methods

- GARK: flexibile theory for solving order conditions
- Construct from base inner and outer methods $T_O = \left\{A^O, b^O, c^O\right\}$, where $c_i^O \le c_{i+1}^O$, $i = 1, \ldots, s^O - 1$ and $T_I = \left\{A^I, b^I, c^I\right\}$, where $c_i^I \le c_{i+1}^I$, $i = 1, \ldots, s^I$.
- MIS method formulation solves sub-problem [1]
- RFSMR concept focuses on defining the residual for splitting [4]
  - $r_i = \sum_{j=1}^{i-1} \left(a_{ij}^O - a_{i-1,j}^O\right) f^{\{s\}}\left(\mathbf{k}_j^{\{s\}}\right)$
  - $\frac{\partial \mathbf{k}^{\{f,i\}}}{\partial \tau} = \frac{1}{c_i^O - c_{i-1}^O} r_i + f^{\{f\}}\left(\mathbf{k}^{\{f,i\}}\right), \quad \tau \in \left[\tau_{i,1}, \tau_{i+1,1}\right], i = 2, \ldots, s^O + 1$
  - Final step solution accumulated similarly to stage solutions
- If both T_O and T_I are at least h^3, and T^O satisfies

$$\sum_{i=2}^{s^O} \left(c_i^O - c_{i-1}^O\right) \left(e_i + e_{i-1}\right)^\intercal A^O c^O + \left(1 - c_{s^O}^O\right) \left(\frac{1}{2} + e_{s^O}^\intercal A^O c^O\right) = \frac{1}{3}, \quad (1)$$

then the MIS method is h^3.

Relaxed Multirate Infinitesimal Step (RMIS) Methods compared

- New method: RMIS
  - Uses same sub-problems as MIS
  - $r_i = \sum_{j=1}^{i-1} \left(a_{ij}^O - a_{i-1,j}^O\right) f^{\{s\}}\left(\mathbf{k}_j^{\{s\}}\right)$
  - $\frac{\partial \mathbf{k}^{\{f,i\}}}{\partial \tau} = \frac{1}{c_i^O - c_{i-1}^O} r_i + f^{\{f\}}\left(\mathbf{k}^{\{f,i\}}\right), \quad \tau \in \left[\tau_{i,1}, \tau_{i+1,1}\right], i = 2, \ldots, s^O + 1$
  - Preserves linear invariants
  - Final step solution accumulated by using only fast stage values at the stage times the slow function is evaluate

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  - $\frac{\partial \mathbf{k}^{\{f,i\}}}{\partial \tau} = \frac{1}{c_i^O - c_{i-1}^O} r_i + f^{\{f\}} \left(\mathbf{k}^{\{f,i\}}\right), \quad \tau \in \left[\tau_{i,1}, \tau_{i+1,1}\right], i = 2, \ldots, s^O + 1$
  - Preserves linear invariants
  - Final step solution accumulated by using only fast stage values at the stage times the slow function is evaluate
- Comparatively, choose:

$$\mathbf{b}_{\mathtt{MIS}}^{\{f\}\intercal} = \begin{bmatrix} c_2^O b^{I\intercal} & \left(c_3^O - c_2^O\right) b^{I\intercal} & \cdots & \left(1 - c_{s^O}^O\right) b^{I\intercal} \end{bmatrix}$$

$$\mathbf{b}_{\mathtt{RMIS}}^{\{f\}\intercal} = \begin{bmatrix} b_1^O \mathbf{e}_1^\intercal & b_2^O \mathbf{e}_1^\intercal & \cdots & b_{s^O}^O \mathbf{e}_1^\intercal \end{bmatrix} \in \mathbb{R}^{s^O s^I} = \mathbb{R}^{s^f}.$$

$$\text{where } \mathbf{e}_1^\intercal = \begin{bmatrix} 1 & 0 & \cdot & 0 \end{bmatrix} \in \mathbb{Z}^{s^I}$$

Simplification of RMIS Order Conditions

Lemma (Sexton & Reynolds, 2018)

Choosing $\mathbf{b}^{\{f\}} = \mathbf{b}^{\{f\}}_{RMIS}$, *and assuming* T_I *has explicit first stage, then:*

$$\begin{aligned}
\mathbf{b}^{\{f\}\intercal}\left(\mathbf{c}^{\{f\}}\right)^q &= \mathbf{b}^{\{s\}\intercal}\left(\mathbf{c}^{\{s\}}\right)^q, \; q = 0, 1, \ldots, \\
\mathbf{b}^{\{f\}\intercal}\mathbf{A}^{\{f,f\}} &= \mathbf{b}^{\{s\}\intercal}\mathbf{A}^{\{s,f\}}, \\
\mathbf{b}^{\{f\}\intercal}\mathbf{A}^{\{f,s\}} &= \mathbf{b}^{\{s\}\intercal}\mathbf{A}^{\{s,s\}}, \\
\left(\mathbf{b}^{\{f\}} \times \mathbf{c}^{\{f\}}\right)^\intercal \mathbf{A}^{\{f,f\}} &= \left(\mathbf{b}^{\{s\}} \times \mathbf{c}^{\{s\}}\right)^\intercal \mathbf{A}^{\{s,f\}}, \\
\left(\mathbf{b}^{\{f\}} \times \mathbf{c}^{\{f\}}\right)^\intercal \mathbf{A}^{\{f,s\}} &= \left(\mathbf{b}^{\{s\}} \times \mathbf{c}^{\{s\}}\right)^\intercal \mathbf{A}^{\{s,s\}}.
\end{aligned}$$

Hence, all of the fast fourth order conditions are equivalent to their slow counterparts, reducing the 28 total conditions to just 14.

We anticipate a similar result for the fifth order conditions ($86 \rightarrow 43$), but have yet to perform the analysis.

RMIS Method Order

Theorem (Sexton & Reynolds, 2018)

Assume that T_I is at least third order. Assume that T_O is explicit, at least fourth order, and satisfies

$$v^{O\intercal} A^O c^O = \frac{1}{12}, \tag{2}$$

where

$$v_i^O = \begin{cases} 0, & i = 1, \\ b_i^O \left(c_i^O - c_{i-1}^O\right) + \left(c_{i+1}^O - c_{i-1}^O\right) \sum_{j=i+1}^{s^O} b_j^O, & 1 < i < s^O, \\ b_{s^O}^O \left(c_{s^O}^O - c_{s^O-1}^O\right), & i = s^O, \end{cases}$$

then the coefficients coefficients $\mathbf{A}^{\{f,f\}}$, $\mathbf{A}^{\{f,s\}}$, $\mathbf{A}^{\{s,f\}}$, $\mathbf{A}^{\{s,s\}}$ and $\mathbf{b}^{\{s\}}$ satisfy all of the "slow" fourth-order conditions.

Condition (2) is analagous to (1), that guarantees the MIS method is h^3.

RMIS & MIS Order Summary

Combining these two results with the existing MIS method theory, we have:

MIS: if (a) T_I is h^3, (b) T_O is explicit and h^3, and (c) T_O satisfies (1), then the MIS method is h^3.

RMIS: if (a) T_I is h^3 and has explicit first stage, (b) T_O is explicit and h^4, and (c) T_O satisfies (2), then the RMIS method is h^4.

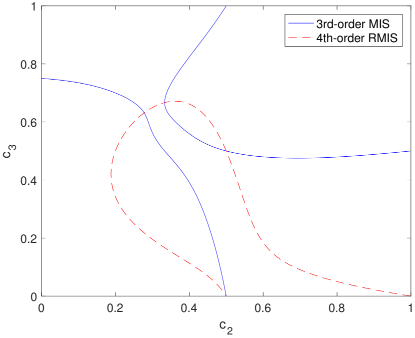
Finally, since MIS and RMIS only differ in their selection of $\mathbf{b}^{\{f\}}$, then if all of the above assumptions are satisfied, we may use MIS as an h^3 *embedding* for the h^4 RMIS method.

Choosing Base Methods

- Represent 4-stage 4th order RK method in terms of stage times c_2 and c_3
- Solve RFSMR and RMIS order condition on the outer/slow base method

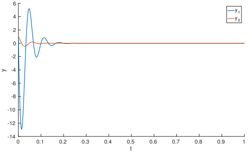
$$\texttt{3/8 - Rule:}\quad \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ \frac{2}{3} & -\frac{1}{3} & 1 & 0 & 0 \\ 1 & 1 & -1 & 1 & 0 \\ \hline & \frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8} \end{array}$$

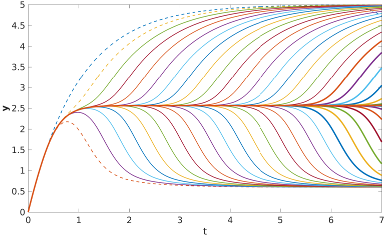
$$\texttt{KW3:}\quad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{3}{4} & -\frac{3}{16} & \frac{15}{16} & 0 \\ \hline & \frac{1}{6} & \frac{3}{10} & \frac{8}{15} \end{array}$$

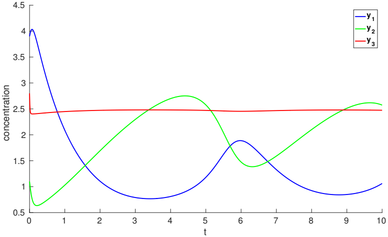


Numerical order and efficiency results

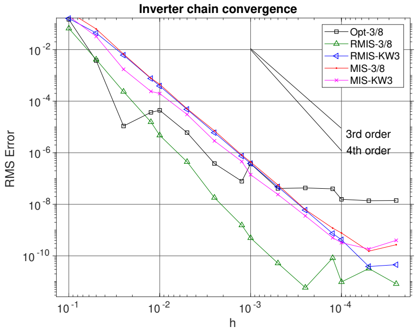
- Test Problems
  - Inverter-chain: weakly coupled, literature [3]
  - Kuhn stability: strongly coupled, linear [2]
  - Brusselator: chemical reaction network, nonlinear [?]
- Methods
  - RMIS w/ 4-stage Base (4th)
  - RMIS w/ 3-stage Knoth-Wolke (3rd)
  - RFSMR w/ 4-stage Base (3rd)
  - RFSMR w/ 3-stage Knoth-Wolke (3rd)

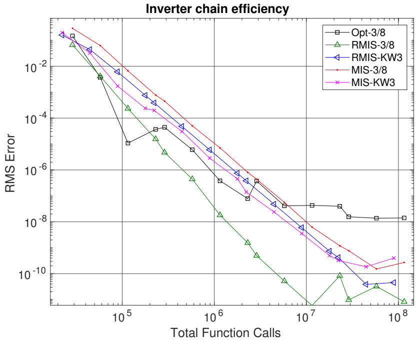






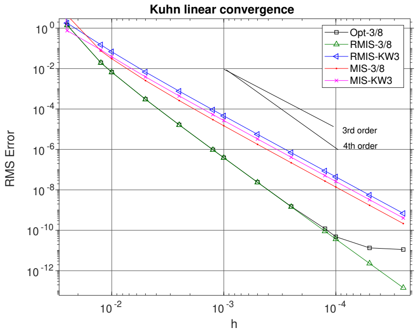
Inverter-chain test results

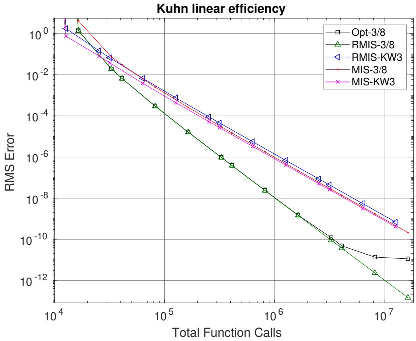




- Fixed step h
- Efficiency horizontal shift depends on number of stages in base method
- RMS error $\sqrt{\sum_{i=1}^{n} \frac{(\hat{\mathbf{y}}_i - \mathbf{y}_i)^2}{n}}$ where $\hat{\mathbf{y}}$ from high order implicit solve with tiny h

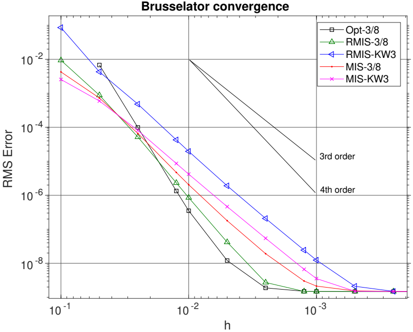
Kuhn stability test results

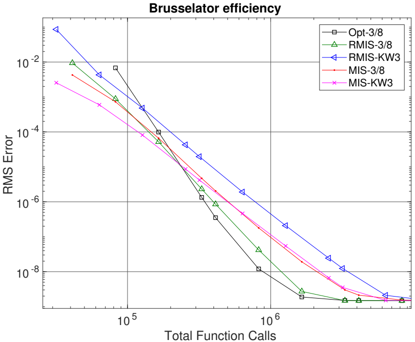




- Fixed step h
- Numerical order and efficiency results are cleaner for this 2×2 linear problem
- RMS error $\sqrt{\sum_{i=1}^{n} \frac{(\mathbf{ytrue}_i - \mathbf{y}_i)^2}{n}}$ where **ytrue** is exact solution

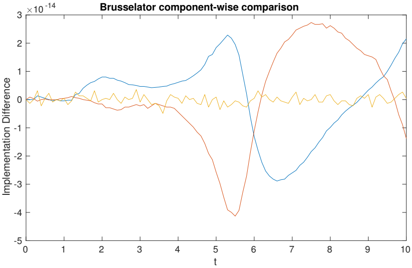
Brusselator test results

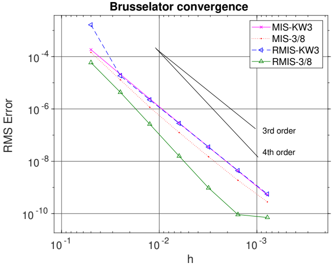




- With fixed step h, our new methods are more efficient for stronger error requirements
- RMS error $\sqrt{\sum_{i=1}^{n} \frac{(\hat{\mathbf{y}}_i - \mathbf{y}_i)^2}{n}}$ where $\hat{\mathbf{y}}$ from high order implicit solve with tiny h

Software





- An updated implementation can be found at https://drreynolds@bitbucket.org/drreynolds/rmis.git
- Testing the RMIS-3/8 method with this new implementation on the Brusselator problem shows close to round-off absolute error differences
- The same convergence properties are observed

Conclusions

- The Generalized-structure Additively-partitioned Runge Kutta can be used in creating new methods based on Multirate Infinitesimal Step Methods with desirable properties
- Using one of our coupling approaches with a base method that also satisfies the slow coupling conditions is a fourth order overall method.
- These multiple coupling approaches allows for approximations of local error by using them together.
- Future areas of interest include:
  - Time-step adaptivity for the slow-time scale based on embeddings
  - Time-step adaptivity for the time-scale ratio based on embeddings
  - Investigate extensions to allow implicitness at the slow time scale
  - Extensions to fifth order (or higher)

Acknowledgements & Questions

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GARK Fifth Order Conditions

The h^5 conditions are, for $\sigma, \nu, \mu, \lambda \in f, s$:

$$\mathbf{b}^{\{\sigma\}\intercal}\left(\mathbf{c}^{\{\sigma\}}\right)^4 = \frac{1}{5} \qquad \text{[2 conditions]},$$

$$\left(\mathbf{b}^{\{\sigma\}} \times \left(\mathbf{c}^{\{\sigma\}}\right)^2\right)^\intercal \mathbf{A}^{\{\sigma,\nu\}}\mathbf{c}^{\{\nu\}} = \frac{1}{10} \qquad \text{[4 conditions]},$$

$$\left(\mathbf{b}^{\{\sigma\}} \times \mathbf{c}^{\{\sigma\}}\right)^\intercal \mathbf{A}^{\{\sigma,\nu\}}\left(\mathbf{c}^{\{\nu\}}\right)^2 = \frac{1}{15} \qquad \text{[4 conditions]},$$

$$\left(\mathbf{b}^{\{\sigma\}} \times \mathbf{c}^{\{\sigma\}}\right)^\intercal \mathbf{A}^{\{\sigma,\nu\}}\mathbf{A}^{\{\nu,\mu\}}\mathbf{c}^{\{\mu\}} = \frac{1}{30} \qquad \text{[8 conditions]},$$

$$\mathbf{b}^{\{\sigma\}\intercal}\left(\mathbf{A}^{\{\sigma,\nu\}}\mathbf{c}^{\{\nu\}}\right)^2 = \frac{1}{20} \qquad \text{[4 conditions]},$$

$$\mathbf{b}^{\{\sigma\}\intercal}\mathbf{A}^{\{\sigma,\nu\}}\left(\mathbf{c}^{\{\nu\}}\right)^3 = \frac{1}{20} \qquad \text{[4 conditions]},$$

$$\mathbf{b}^{\{\sigma\}\intercal}\mathbf{A}^{\{\sigma,\nu\}}\left(\mathbf{c}^{\{\nu\}} \times \left(\mathbf{A}^{\{\nu,\mu\}}\mathbf{c}^{\{\mu\}}\right)\right) = \frac{1}{40} \qquad \text{[8 conditions]},$$

$$\mathbf{b}^{\{\sigma\}\intercal}\mathbf{A}^{\{\sigma,\nu\}}\mathbf{A}^{\{\nu,\mu\}}\left(\mathbf{c}^{\{\mu\}}\right)^2 = \frac{1}{60} \qquad \text{[8 conditions]},$$

$$\mathbf{b}^{\{\sigma\}\intercal}\mathbf{A}^{\{\sigma,\nu\}}\mathbf{A}^{\{\nu,\mu\}}\mathbf{A}^{\{\mu,\lambda\}}\mathbf{c}^{\{\lambda\}} = \frac{1}{120} \qquad \text{[16 conditions]}.$$

Subcycling as a One-Step Method

Consider taking 3 substeps of size $\frac{h}{3}$ with the midpoint method,

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1 \end{array} = \begin{array}{c|c} c & A \\ \hline & b^{\mathsf{T}} \end{array}:$$

Basic steps

$$\begin{aligned} z_1 &= y_n \\ z_2 &= y_n + \tfrac{h}{6} f(z_1) \\ y^* &= y_n + \tfrac{h}{3} f(z_2) \end{aligned}$$

$$\begin{aligned} z_3 &= y^* \\ z_4 &= y^* + \tfrac{h}{6} f(z_3) \\ y^{**} &= y^* + \tfrac{h}{3} f(z_4) \end{aligned}$$

$$\begin{aligned} z_5 &= y^{**} \\ z_6 &= y^{**} + \tfrac{h}{6} f(z_5) \end{aligned}$$

$\rightarrow$

Single step

$$\begin{aligned} z_1 &= y_n \\ z_2 &= y_n + \tfrac{h}{6} f(z_1) \\ z_3 &= y_n + \tfrac{h}{3} f(z_2) \\ z_4 &= y_n + \tfrac{h}{3} f(z_2) + \tfrac{h}{6} f(z_3) \\ z_5 &= y_n + \tfrac{h}{3} f(z_2) + \tfrac{h}{3} f(z_4) \\ z_6 &= y_n + \tfrac{h}{3} f(z_2) + \tfrac{h}{3} f(z_4) \\ &\quad + \tfrac{h}{6} f(z_5) \end{aligned}$$

$$y_{n+1} = y_n + \tfrac{h}{3} f(z_2) + \tfrac{h}{3} f(z_4) + \tfrac{h}{6} f(z_6)$$

$\rightarrow$

Butcher tableau

$$\begin{array}{c|cccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{2}{6} & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 \\ \frac{3}{6} & 0 & \frac{1}{3} & \frac{1}{6} & 0 & 0 & 0 \\ \frac{4}{6} & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 \\ \frac{5}{6} & 0 & \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{6} & 0 \\ \hline & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} \end{array}$$

$$\Updownarrow$$

$$\begin{array}{c|ccc} \frac{1}{3}c & \frac{1}{3}A & 0 & 0 \\ \frac{1}{3}1 + \frac{1}{3}c & \frac{1}{3}1b^{\mathsf{T}} & \frac{1}{3}A & 0 \\ \frac{2}{3}1 + \frac{1}{3}c & \frac{1}{3}1b^{\mathsf{T}} & \frac{1}{3}1b^{\mathsf{T}} & \frac{1}{3}A \\ \hline \end{array}$$